

Survival Guide for Graduate Students in Scientific Computation

Chris Danforth
danforth@math.umd.edu

Danny Dunlavy
ddunlavy@cs.umd.edu

Aaron Lott
palott@ipst.umd.edu

Bob Shuttleworth
rshuttle@math.umd.edu

Fall 2005

Abstract

The Scientific Computation (SC) Concentration has recently been added to the Applied Mathematics and Scientific Computation (AMSC) Program at the University of Maryland, College Park. Although there is a list of requirements for the SC Concentration which helps guide students through their program, there is a great deal of flexibility (for good reasons and to the benefit of the students) and there is less precedence and experience that current and future students can rely upon than there is for students in the Applied Mathematics (AM) Concentration.

We hope that this document answers some of the general questions students may have about the SC Concentration. Specifically, any student enrolled in or interested in the AMSC Program and enjoys solving problems using computation and simulation should read this document to get a student's perspective on the SC Concentration.

Contents

1	Introduction	2
2	The Road to Candidacy	2
2.1	Orientation	2
2.2	Study Advisory Committee Report	3
2.3	Coursework	4
2.4	Candidacy Oral Examination	7
2.5	Summertime	8
3	Resources	10
3.1	Online Materials	10
3.2	Computational Tools	11
3.3	Computational Facilities	11
3.4	Seminars	11
4	Opportunities	12
4.1	Participation	12
4.2	Leadership	13

1 Introduction

This document is intended to act as a primer for students interested in the Scientific Computation (SC) Concentration of the Applied Mathematics and Scientific Computation (AMSC) Program at the University of Maryland, College Park. However, some material presented here may be of interest to students in the Applied Mathematics (AM) Concentration as well, especially in Section 4, which contains information about activities and funding opportunities.

This document is intended for incoming students as it contains information that is important to know (or at least to think about) during Orientation before the first semester of coursework. However, students should consult this guide throughout their time in the program for several reasons. In order for a program to be as strong and as lasting as it can be, support and leadership from the student body is essential. However, this is easier said than done. By the time students are in a position to help, they are often finishing up their work in the program and are on their way out. We hope that future students will take time out of their busy schedules to amend this document to address the needs and concerns of the students of the Scientific Computation Concentration.

There are many differences between the AM and SC Concentrations. The most striking difference is that the qualifying requirements for the two programs differ quite drastically. More importantly, the differences in these requirements reflect the differences in the needs, interests, and goals of the students in the two Concentrations. The SC Concentration has been designed for students interested in developing algorithms and software systems which use mathematical techniques in solving problems in the sciences. For students interested in developing computational skills through their coursework, the SC Concentration may be a better choice than the AM Concentration. It is certainly possible, though, for students in the AM Concentration to pursue a course of study to this end, but a discussion of such pursuit is beyond the scope of this document.

We admit that this guide is geared toward those students pursuing a Ph.D., but this should not deter students pursuing a master's degree from reading it, or possibly even adding a section or two containing information specific to the M.S. degree (hint, hint).

2 The Road to Candidacy

There are several milestones that you need to pass along your way to advancing to candidacy, and we have attempted to highlight those here. It is possible to advance to candidacy as early as the summer following your second year, but must be completed by March 1 of your fourth year to maintain TA support from the Mathematics Department and by the end of your fifth year in order to remain in the program.

2.1 Orientation

This is a crucial time for students in the Ph.D. program. So much information has to be processed— new names and faces, forms to be filled out, room assignments, keys to get, pictures to take, computer accounts to access— it's easy to forget to think about what you want to do with your time here and how to accomplish these goals. You may think that this can wait until later— at least until the second semester. However, for students interested in the SC Concentration there are decisions that need to be made *before* your first class that either may affect your funding or at least delay your coursework by a full academic year.

Students interested in the SC Concentration should take the Core Courses starting in the Fall Semester of the first year. A recommended schedule of these courses are as follows:

<i>Core Course</i>	<i>Timeline</i>
AMSC 660 SC I	Year 1, Fall
AMSC 661 SC II	Year 1, Spring
AMSC 662 COPSC	Year 1/2, Fall
AMSC 663 Adv. SC I	Year 2, Fall
AMSC 664 Adv. SC II	Year 2, Spring

The AMSC 660-1 sequence must be taken before the AMSC 663-4 project course. Furthermore, in the past, AMSC 661 has only been offered in the Spring Semester. Therefore, if a student does not take AMSC 660

in the Fall Semester during the first year, the earliest date the Core Courses could be completed would be the end of the student's third year. However, the requirements for remaining in the AMSC Program as a full time student as well as maintaining TA support from the Mathematics Department specify that these courses *must be completed by the end of the student's second year*.

Most students are assigned a seasoned graduate student to act as a mentor during orientation. If there are questions you have about courses and the requirements of the SC Concentration, ask your student mentor or the authors of this document, as they are most likely well versed in the requirements since they are currently navigating through the AMSC Program themselves.

Other things to do if time permits (many of these are described in greater detail throughout the remainder of this document):

- Visit the AMSC web site (<http://www.amsc.umd.edu/>).
- Visit the SC Student Site (<http://www.cscamm.umd.edu/scstudents/>).
- Visit CSCAMM and IPST and talk to the AMSC students there
- Talk to your advisor or an AMSC faculty member who advises SC students about the SC Concentration

2.2 Study Advisory Committee Report

The Study Advisory Committee (SAC) report is designed to demonstrate you are on track to satisfy the requirements of your chosen concentration. This document determines your TA renewal, when you can apply to advance to candidacy, etc. Simply stated, this document is a list of the courses you have taken, and those you will take to fulfill the requirements of the AMSC Program. For those in the SC Concentration, one is required to pass AMSC 660-664 and six (6) graduate credits of core science courses with a GPA of 3.5 or higher. Additionally, six (6) graduate credits of scientific application level courses and nine (9) hours of electives must be passed with a grade of B or higher.

You should begin a draft of this report as soon as you arrive at UM (keep in mind that your SAC is a work in progress and can change) , and you should submit a final copy as soon as you have chosen a scientific application. This plan should detail the semesters during which you will take the specific core science and applications courses, as well as any other coursework relevant to your discipline. Once you have completed the SAC report, available at the AMSC Office, it must be signed by the three AMSC Faculty. At least one of these faculty members must be from your area of application. If you have an advisor, ask them to help you choose your committee. If you don't have an advisor, ask a senior SC graduate student to help you. The function of this committee is to ensure that your plan of coursework will satisfy the degree requirements. The report will then be evaluated by the AMSC Graduate Committee during their next meeting. If the report is approved, it becomes a contract ensuring the outlined course of action will satisfy the preliminary qualifications of the SC concentration.

In the event that your area of interest should change after your SAC report has been approved, the report can be resubmitted. It is important that you attempt to draft a SAC report as early as possible, even during orientation with the help of your mentor or senior SC grad student. Samples of SAC reports that have been approved by the AMSC Graduate Committee will be available on the SC Student Site: (<http://www.cscamm.umd.edu/scstudents/>). These are examples of successful paths, but are by no means the only route to qualifying. Be creative.

2.3 Coursework

A recommended schedule for satisfying the core course requirements for the SC Concentration is outlined in section 2.1. Each SC student must also apply computational methods in a scientific discipline outside of AMSC/MATH by completing two core science course focusing on theory and two applications courses focusing on computational methods important to solving problems in the discipline.

AMSC 660/661

These courses, Scientific Computing I and II, are two of the five core scientific computing courses offered at UM. These courses provide background in Monte Carlo simulation, numerical linear algebra, nonlinear systems, optimization, ordinary differential equations and partial differential equations. The fundamental computational techniques and software packages used in scientific computation are covered, with only an introduction to the theory presented.

AMSC 662

This course, Computer Organization and Programming for Scientific Computing, is one of the five core scientific computing courses offered at UM. This course presents fundamental issues of computer hardware, software, parallel computing, and scientific data management for developing code for scientific computation. In the past, it has been a traditional lecture-style course with several programming assignments and exams. The majority of assignments have been more in line with those found in computer science courses than those in mathematics courses.

AMSC 663/664 - Project Course

The project course is a year long course in which each student develops software for a scientific task in a high performance computing environment. This project does not have to be a thesis project or even related to what you want to do for your thesis. However, it is computational in nature (with the theoretical issues already completed worked out by *someone else*) and must be written in some high level programming language (C/C++, JAVA, Fortran, etc). The greatest pitfall with this course is getting started. Finding an advisor for this project can be tedious and in some cases frustrating. Try to find an advisor as early as possible, preferably in the summer before your second year in the SC Concentration. This will allow you to start on your project sooner and get more out of the course sequence. If there is an area in which you are interested and you are having trouble finding an advisor, feel free to ask past students or class instructors about potential project advisors. Also, go to various seminars/lectures/talks offered in departments at UM; these are good places to find potential advisors.

We recommend that you are well acquainted with your application science when the course begins. We implore you to have an advisor chosen WELL before the course begins! In the past, successful projects have resulted from good preparation during the months before 663 meets for the first time.

SC students may choose a problem that will eventually become their thesis work, but it is not a requirement. Some students choose to use the project course to examine a problem completely unrelated to their application area. Masters students who complete a thesis need not take the project course. Projects from past years can be found on the SC Student Site (<http://www.cscamm.umd.edu/scstudents/projects/>).

Core Science Courses

SC students must take two (2) graduate-level core science courses, designed to expose students to the fundamental theory of their chosen discipline. These courses cannot be offered or cross-listed by the Mathematics or Computer Science Departments, but rather should come from Engineering, Business, Physics, or some other AMSC Affiliate Department. A list of courses from that past SC students have chosen to fulfill this requirement are available on the SC Student Site (<http://www.cscamm.umd.edu/scstudents/courses/>).

Scientific Application Courses

SC students in the Ph.D. Program must complete two graduate level applications courses intended to expose students to the computational methods relevant to their chosen discipline (M.S. students need only one). A list of courses from that past SC students have chosen to fulfill this requirement are available on the SC Student Site: (<http://www.cscamm.umd.edu/scstudents/courses/>).

Electives

SC students in the Ph.D. Program must also take three (3) electives (MS students 2). It may be wise to use these courses to gain a breadth of knowledge in computational methods or areas in which you are interested outside of your project or thesis areas. You may find that you do not have the time to focus on these areas once you start to focus on your thesis work.

Remarks

Although other SC students can present you with lists of courses they have taken or they know have been part of other students' training, your advisor is the best source of information on which courses will best prepare you for your thesis work. Spending time in the first year of graduate school trying to narrow your focus on application areas that interest you will help you choose your courses as well.

2.4 Candidacy Oral Examination

In order to advance to candidacy, students must complete all of the qualifying requirements: completion of the Core Courses and Core Science Courses with a minimum GPA of 3.5 in those courses. Keep in mind that you must get at least four A's in these seven courses (for now, the +/- attached to the grade does not change the grade points earned: A=4, B=3). Also, you are not allowed to get less than a B- in these courses.

You must also write a research proposal called a prospectus, which is described below. You must get three AMSC Faculty to serve on your examination committee, and sign that your prospectus is acceptable. The AMSC Graduate Committee also must approve your prospectus before your examination. Therefore, the process of writing and editing your prospectus, along with the approval process may take several months to complete. Keep this in mind to make sure that you dedicate enough time for writing, that faculty members are around (e.g., during summer months), and that you plan your timeline around the AMSC Graduate Committee meeting times (which usually only occur once per semester) with enough spare time to accommodate any unforeseen setbacks.

Once your prospectus has been approved, you are free to schedule your Candidacy Oral Exam with your committee at any time. However, you should make sure you respect the busy schedules of your committee members. Suggest several options for meeting times that are at least a week or two in the future. Do not expect that all of your committee members will be available during the summer months. Finally, if after several attempts at scheduling a meeting time you are not able to set a time with your committee members, ask the Chair of your committee to step in and help.

With these thoughts in mind, we now turn to the writing and editing of the prospectus.

Prospectus

For your Candidacy Oral Examination, you write a prospectus defining the areas to be covered. The prospectus covers an application area or open problem in an application area. Since SC students must complete their project course before this examination, the area of the student's project is most likely an ideal area to be covered. The prospectus must list relevant courses taken as well as book chapters and papers important to the area or problem. When choosing to include references in your prospectus, make sure you understand the material well, as anything included in the list of references can be covered during the examination. Be sure to read the instructions included in the form for the examination available from the AMSC Office before attempting to write your prospectus, as they specify the information that is required to be included in the prospectus.

You should work closely with your advisor while writing your prospectus, as this person will be the Chair of your Examination Committee. You should verify which book chapters and papers are important to include as well as ask what types of questions you should expect during the examination. Advice differs from advisor to advisor, but a good goal for a first draft of your prospectus should be 4-6 pages.

During the first part of your examination, you present the material covered in your prospectus. This does not mean that you should just cut and paste paragraphs from the prospectus onto several slides. Again, advice differs, but prepare the presentation as if you were going to give a conference talk (only a bit longer) or a seminar talk (only a bit shorter). After your presentation, the floor is open to questions from the Examination Committee.

Samples of prospectuses and presentations written by SC students for their Candidacy Oral Examinations are available on the SC Student Site (<http://www.cscamm.umd.edu/scstudents/docs/prospectus/>).

2.5 Summertime

Summer is a time to relax with no classes and humid weather, but it serves as a golden opportunity to have experiences that will help enhance your resume and broaden your future prospects. For graduate students completing their first year, the first summer is a perfect time to look for and choose a topic for the 663/664 project course.

The summer break is an excellent opportunity for graduate students to explore future prospects, including employment. If a summer opportunity/internship is positive, then great, it could lead to a topic for the AMSC 663-664 project course or a refereed paper. In terms of funding and finances, it could lead to a fellowship, research assistantship (RA), or even a full-time position after graduation. Some employers provide chances to participate in conferences or seminars that allow one to present your work or publish a technical report or even refereed journal article.

On the other hand, not all opportunities or internships are worthwhile. However, this too can be a positive experience because it allows one to figure out what types of research/problems one enjoys. For example, a summer experience in private industry may help one realize that the deadlines and corporate structure is not for them, but rather teaching in a university setting is more what one is seeking.

Opportunities and internships abound in the College Park area. Below are a few opportunities broken down into four entities (Opportunities at UM, those in government facilities, private industry, and various summer schools). Talk to other graduate students to get a feel for how to apply and how experiences at these locations were.

UM

At the University of Maryland, there are three major areas that provide summer support. They are teaching assistantships, research assistantships, and teaching institutes. The Computer Science and Mathematics Departments provide summer support in the form of teaching assistantships. In Mathematics, the jobs range from grading homework/tests in undergraduate courses, teaching courses as the sole contact instructor, or proctoring Math Placement Exams for incoming first year students and transfer students. Normally, letters and e-mails appear around April for these opportunities. There are also a number of summer teaching institutes, these include summer camps for gifted and talented high school students. Information about these opportunities normally appear around late March or early April in the form of e-mails published by the Mathematics Department.

Research assistantships (RAs) abound during the summer. These types of opportunities can be very worthwhile for a graduate student completing their first year of graduate school. If a problem is interesting enough, it can serve as a launching pad for a topic in the project course (AMSC 663-664). In turn, this may lead to a thesis topic or a paper detailing your summer findings. Finding an appropriate RA can be a bit tricky due to the interdisciplinary nature of the AMSC Program. Summer RAs abound in all departments, including Mathematics, Computer Science, and the many of the engineering departments. One excellent way to find an appropriate topic is by asking around, and consulting other grad students. An even better resource can be found by asking professors that teach the core science courses or other courses in which you are interested. Even if these instructors do not have summer RA positions available, one of their colleagues may.

National Research Facilities

Summer opportunities at national research facilities are abundant. Past SC students have held positions at many government research labs. These include: National Institutes of Health (NIH), National Aeronautical and Space Administration (NASA), National Institute of Standards and Technology (NIST), National Security Agency (NSA) DOE's Sandia National Laboratory, DOE's Los Alamos National Laboratory, DOE's Oak Ridge National Laboratory, and Department of Defense Research labs. For some of these opportunities, security clearances are required, so one should start looking for and applying for positions no later than November. Several AMSC students work at these facilities, so by talking to senior students and by paying attention to email from faculty members one can learn how to get an internship from these institutions.

Private Industry

The need for high performance computing has grown significantly in the past few years. Summer jobs at consulting firms (Booz-Allen/Institute for Defense Analyses (IDA)), pharmaceutical companies (Pfizer/Merck), financial firms (World Bank/Merrill Lynch), aerospace firms (Boeing), and oil firms (Shell/BP) have been available in the past.

Summer Schools

The Institute for Mathematics and its Applications (IMA) offers many interesting summer schools that can be used as a springboard for a dissertation or topic for the project course. The University of Maryland is a contributor to the IMA, so graduate students are encouraged and entitled to attend (i.e., funding is available) some of the various, in-depth summer schools offered each summer by the IMA. Check the IMA web site for more information (<http://www.ima.umn.edu/>).

There are also opportunities at the Mathematical Sciences Research Institute (MSRI) in Berkeley, CA. The University of Maryland is also a contributor to the MSRI, and so graduate students can receive funding to participate in the summer programs offered there. A list available programs is available on their web site (<http://www.msri.org/>).

The Industrial Mathematical & Statistical Modeling Workshop for Graduate Students at North Carolina State University is an opportunity to meet and work with graduate students from other institutions as well as with professionals from industry. Deadlines are in early April for the following summer. Go to the Workshop's web site for more details (<http://www.ncsu.edu/crsc/ims/>).

3 Resources

In this section we give a brief introduction into the resources available to SC students.

3.1 Online Materials

AMSC

This is the official site of the AMSC Program. Links to Faculty and Student email addresses are provided as well as useful to facilitate research, including application areas of AMSC Faculty members (<http://www.ams.umd.edu/>).

SC Student Site

The SC Student Site (<http://www.cscamm.umd.edu/scstudents/>) is maintained by students with information for students in the SC Concentration as well as students at UM interested in scientific computation in general. This site serves as a central repository of the following information:

- List of of interest to SC students (seminars, tools, facilities, etc.)
- Past SC student projects, prospectuses, and presentations
- Links to SC-affiliated faculty web pages
- Funding opportunities

SC Student Listserv

The SC Student Listserv (scstudents@listserv.umd.edu) serves as a medium to share information regarding the SC program. Regular posts are made informing the community of upcoming events, and scientific computation related issues. Discussions pertaining to scientific computation are welcome.

To join the list, go to <http://www.listserv.umd.edu/archives/scstudents.html> and click on the link that says, "Join or leave the list (or change settings)".

3.2 Computational Tools

CMPS has a site license for Matlab and Mathematica. Students can obtain a copy of these products from the Math department's help desk. Those who wish to use Matlab off-campus will need to download a campus VPN client (<http://www.helpdesk.umd.edu/topics/applications/vpn/3836/>) clients are provided for Linux 2.2 kernel, Solaris, MacOS 8 and higher, as well as Windows 98 and higher.

3.3 Computational Facilities

There are several computational facilities on campus available to SC students. Several research groups have their own Beowulf cluster, and/or access to supercomputers at National Laboratories. Both UMIACS and IPST have several Beowulf Clusters (<http://www.lcv.umd.edu/cluster>) and CSCAMM houses an 8 node IBM SP2 cluster (<http://www.cscamm.umd.edu/facilities/computing/sp2/index.htm>).

3.4 Seminars

There are several seminars both on and off campus. Seminars give students a chance to meet potential advisers, and become involved in research projects. They give students an opportunity to meet many people with similar interests. Showing up, and asking questions puts new students on the radar. It is in the students interest to start attending seminars right away even though one might not understand much in the beginning. However, attending the seminars will give students the chance to learn lecturer styles, and the format of technical talks.

SC Student Seminar

The main focus of this seminar will be to give SC students a chance to give talks on their research, as well as broaden the SC student knowledge base in topics of Scientific Computing. We plan to invite occasional guest speakers to give lectures on topics of interest.

Other Seminars

Applied Math/PDE, Numerical Analysis, CSCAMM, IPST, Dynamical Systems, UMIACS, CS, and the Distinguished Lectures Series. Dates, times and titles of talks are sent out via departmental mailing lists each week.

4 Opportunities

There are many opportunities on campus (and slightly off campus at NIH, NIST, etc) for students to give talks, posters, and interact with other students in organized scholarship activities. Here are a few areas that we chose to highlight:

4.1 Participation

RIT

Research Interaction Teams (RIT) are designed to ease the transition from coursework to research. These are informal (once a week) meetings driven by faculty, but have lots of interaction from students. These allow students to work on "real" problems and are a good opportunity to look at possible advisors. A list of the current RITs can be found on the Mathematics Department web site (<http://www.math.umd.edu/graduate/current/RITs.shtml>).

Spotlight on Graduate Research

The Spotlight on Graduate Research event (<http://www.math.umd.edu/research/spotlight/>) is designed to give graduate students working on research projects the opportunity to practice presenting material to a general mathematical audience and to communicate the types of research being done by students. It is open to graduate students currently enrolled in the MATH, AMSC, and STAT programs.

Benefits include:

- Opportunity to give 20-minute technical talk to peers
- Cash prizes available (4 prizes of \$250 each in the past)

The event usually takes place in the Fall Semester, with 4 finalists giving 50-minute versions of their talk in the Spring Semester.

GRID

Run by the Graduate Student Government (GSG), Graduate Research Interaction Day, or GRID (<http://www.gsg.umd.edu/GRID>), is a one-day inter-disciplinary poster competition and a graduate student networking event for students to showcase their research and network with students and faculty from different departments.

Benefits include:

- Great opportunity to present your work to a broad audience
- Cash prizes available (up to \$500)
- UM T-shirts given to all participants
- GSG pays to print your poster in large, glossy format

GRID usually takes place in April each year, with submissions due at the beginning of the month and the poster session taking place at the end of the month.

SIAM

The Society of Industrial and Applied Mathematics, or SIAM (<http://www.siam.org/>) is a professional organization promoting advanced research, career development and networking opportunities for and amongst industry, government, and academic professionals in the area of applied and computational mathematics.

Membership is **free** for students in the AMSC Program. There is also a local chapter at UM that organizes pizza/movie/talk nights.

4.2 Leadership

AMSC Graduate Committee

The AMSC Graduate Committee consists of the AMSC Director, eight AMSC faculty members and a student representative. Among other things, this committee approves SAC Reports and determines passing levels for qualifying examinations. Serving as the AMSC Graduate Committee Student Representative provides one the opportunity to gain experience working on an academic committee, interact with students and faculty to voice student concerns, and help impact policy regarding students.

SC students who have completed all of the Core Courses with a grade-point average of at least 3.5 in those courses are eligible to act as the student representative. The AMSC Graduate Student Representative also serves as a student representative on the Department of Mathematics Graduate Committee and as the President of the AMSC Student Council.

To learn more about the AMSC Graduate Committee and its role in the AMSC Program, read the AMSC Plan of Organization (<http://www.amsc.umd.edu/Faculty/Governance/overview.html>).

AMSC Student Council

The AMSC Student Council (ASC) has been organized to plan and promote educational and social interaction amongst the students in the AMSC Program. Membership is limited to 5 students, with elections held each Spring. The ASC President serves as the Student Representative on both the AMSC Graduate Committee as well as the Department of Mathematics Graduate Committee, and two ASC Members also serve as the AMSC Representatives on the Graduate Student Government (GSG).

To learn more about the ASC and its role in the AMSC Program, visit the ASC web site (<http://www.amsc.umd.edu/Current/asc/>).